

Spin-One Bosons in Low Dimensional Mott Insulating States

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We analyze the strong coupling limit of spin-one bosons in low dimensional lattices. In one-dimensional lattices, for an odd number of bosons per site ($N_0 = 2k + 1$), the ground state is a dimerized valence bond crystal with a two-fold degeneracy; the low lying elementary spin excitations carry spin-one. For an even number of bosons per site ($N_0 = 2k$), the ground state is a nondegenerate spin singlet Mott state. We also argue that in square lattices in a quantum spin disordered limit, ground states should be dimerized valence bond crystals for an odd integer N_0 . Finally, we briefly report results on exotic states for non-integer numbers of bosons per site in one-dimensional lattices.

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Recently, Greiner et al. reported the observation of superfluid and Mott insulating states in optical lattices [1]. The experiment convincingly demonstrates the feasibility of investigating many-body states of cold atoms by varying laser intensities of optical lattices [2,3]. Because of controllable properties of optical lattices, it is now widely accepted that many strong-coupling limits which are not accessible in solid-state systems can be investigated in optical lattices. Furthermore, since optical lattices are free from imperfections, an accurate comparison between theories and future experiments appears to be likely. Consequently, we believe that studies of spin-one atoms in optical environments might also create new opportunities for understanding some fundamental issues in quantum magnetism. This in turn should be useful to possible applications toward quantum information storage and processing.

Spin correlated condensates have been recently investigated in experiments [4,5]; two-body scatterings between spin-one atoms were found to result in either ferromagnetic or antiferromagnetic condensates [6–8]. Due to spin-phase separation there also exist a variety of novel condensates which carry distinct fractionalized topological excitations [9–11]. Interesting spin correlated fractional quantum hall states were also analyzed [12,13].

For spin-one bosons with antiferromagnetic interactions in high dimensional optical lattices, spin correlated Mott insulating states were investigated very recently [10]. Spin singlet and nematic Mott insulators were pointed out for interacting spin-one bosons in strong-coupling and intermediate coupling limit respectively. In this Letter we examine spin correlations in low dimensional Mott insulating states. We show that in the strong-coupling limit in one-dimensional optical lattices, there are two distinct Mott states depending on the "even-odd" parity of numbers of spin-one bosons per site (N_0). When N_0 is an even number, the ground state is a non-degenerate spin singlet Mott state and the lowest lying elementary spin excitations correspond to spin $S = 2$ ones; for an odd integer N_0 , the ground state is a dimerized valence bond crystal which has a two-fold de-

generacy and an elementary spin excitation in this state corresponds to a spin-one state. We also report results for one-dimensional lattices with non-integer numbers of atoms per site and square lattices. To get oriented, let us first consider the following coupled "mesoscopic" spinor condensates.

Two coupled condensates of spin-one atoms

Consider atoms such as sodium ones which interact with each other via antiferromagnetic interactions [6–8]. Assuming all atoms condense to a single one-particle orbital state, we have shown that the dynamics of this condensate is characterized by a constrained quantum rotor model [9–11]. The effective Hamiltonian of two coupled spinor condensates (at site A and B) of spin-one bosons with antiferromagnetic interactions can therefore be expressed as

$$\begin{aligned} \mathcal{H}_{AB} &= \sum_{k=A,B} \frac{\mathbf{S}_k^2}{2I} + \frac{N_k^2}{2C} - N_\alpha \mu + \mathcal{H}_{hop}, \\ \mathcal{H}_{hop} &= -t \mathbf{n}_A \cdot \mathbf{n}_B \cos(\chi_A - \chi_B). \end{aligned} \quad (1)$$

In Eq.1, at each site k two unit vectors \mathbf{n}_k (defined on a two-sphere) and $e^{i\chi_k}$ (defined on a unit circle) characterize the orientation of an $O(3)$ - and $O(2)$ - rotor respectively; they are conjugate variables of the spin operator \mathbf{S}_k and atom number operator N_k , i.e. $[\mathbf{S}_{k\alpha}, \mathbf{n}_{k\beta}] = -i\hbar e_{\alpha\beta\gamma} \mathbf{n}_{k\gamma}$, $[N_k, \chi_k] = i\hbar$. The total spin of a condensate at site k is therefore the angular momentum of the $O(3)$ -rotor at the same site.

\mathcal{H}_{hop} originates from hopping of bosons from one site to other and conserves the total spin of two coupled condensates. t is equal to $N_0 t_0$; t_0 is the hopping integral of an individual boson. t can be varied by changing laser intensities in optical lattices [1]. $E_s = (2I)^{-1} = 4\pi\hbar^2(a_2 - a_0)\rho_0/3MN_0$ and $E_c = (2C)^{-1} = 4\pi\hbar^2(2a_2 + a_0)\rho_0/3MN_0$ characterize the spin and "charge" gaps in the excitation spectrum. They depend on the atomic mass M , the atomic number density ρ_0 and two-body scattering lengths $a_{2,0}$ in the total spin $S = 2, 0$ channels for two spin-one cold atoms. And for sodium atoms, a_2 exceeds a_0 by a few percent [6].

$N_0 (\gg 1)$ is the number of bosons per site and μ is the chemical potential.

Finally, the Hilbert space of the Hamiltonian in Eq.1 is furthermore subject to a constraint $(-1)^{S_k+n_k} = 1$ so that the corresponding microscopic wave functions are symmetric under the interchange of two bosons; S_k, n_k are the eigenvalues of \mathbf{S}_k, N_k respectively (see section II B in Ref. [11] for more discussions on the constraint). We will consider a situation where E_s is much smaller than E_c because the difference between a_2 and a_0 is much smaller than a_0 as for sodium atoms; furthermore in the strong-coupling limit which interests us, t is much smaller than both E_s and E_c .

When the energy gap $E_c (\gg E_s)$ is much larger than the hopping energy t , bosons are localized at each site; and if there are $N_0 = 2k$ bosons at each site and the hopping is absent ($t = 0$), the ground state for each isolated site is an $S = 0$ state where each pair of atoms forms a spin singlet, following Eq.1 and the constraint. This limit was also discussed in [8]. Excitations have to be spin $S = 2, 4, 6, \dots$ states and are gapped by an energy of order of E_s . Therefore, two *weakly* coupled condensates also have a spin singlet ground state and all excitations are gapped by either E_s or E_c . Particularly, there will be no excitations at an energy scale much lower than E_s . In lattices of all dimensions, ground states in this limit are spin singlet Mott insulating states as pointed out in a previous work [10] (see Fig.1a)).

The situation for an odd number of particles per site is more involved. When the hopping is absent, the ground state for each individual site is a spin-one state with a three-fold degeneracy. Eq.1 and the constraint further indicate that excitations are states with spin $S = 3, 5, \dots$ which are gapped from the spin-one ground state. So at energies smaller than E_s , each individual spinor condensate can be treated as a spin-one *pseudo-particle*. For two decoupled sites, the ground state has a nine-fold degeneracy, corresponding to states with total spin $S = 0, 1, 2$.

A detailed calculation, taking into account virtual hoppings between two sites, shows that the effective exchange interaction (for E_s smaller than E_c) is $\mathcal{H}_{AB} = -J \sum_{S=0,1,2} \alpha_S P_S(\mathbf{S}_A + \mathbf{S}_B)$. Here $P_S(\mathbf{S}_A + \mathbf{S}_B)$ is the projection operator of a total spin S state of the two condensates A and B. $J = t^2/E_c$ is the strength of the exchange energy and is much smaller than $E_{c,s}$;

$$\alpha_S = \frac{\gamma_1(S)}{1 - 4c_s} + \frac{\gamma_2(S)}{1 + 2c_s} + \frac{\gamma_3(S)}{1 + 8c_s}, \quad (2)$$

where $\gamma_1(0) = 1/6$, $\gamma_3(0) = 2/15$; $\gamma_3(1) = 1/10$; $\gamma_2(2) = 2/15$, $\gamma_3(2) = 7/150$; $\gamma_2(0) = \gamma_1(1) = \gamma_2(1) = \gamma_1(2) = 0$. $c_s = E_s/E_c$; and α_0 is always larger than $\alpha_{1,2}$.

Eq.2 indicates that two coupled spinor condensates, each of which has $N_0 = 2k + 1$ atoms again have a spin singlet ground state. The lowest lying spin excitations correspond to $S = 2$ ones, whose energies in this case

are equal to $\epsilon(S = 2) = J(\alpha_0 - \alpha_2)$. In addition, there are excitations of spin $S = 1$, with energies $\epsilon(S = 1) = J(\alpha_0 - \alpha_1)$ and $\epsilon(S = 1) > \epsilon(S = 2)$. In the following we will focus on ground states and excitations in low dimensional optical lattices with odd numbers of bosons per site in the strong-coupling limit. The "even-odd" feature emphasised in this letter is absent in the phase diagram for spinless bosons discussed in Ref. [2].

1D lattices with odd numbers of bosons per site

For the study of one-dimensional lattices, we generalize the two-site Hamiltonian in Eq.1 to

$$\mathcal{H}_{1D} = -J \sum_{\langle ij \rangle} \alpha_S P_S(\mathbf{S}_i + \mathbf{S}_j). \quad (3)$$

The sum is over $\langle ij \rangle$, all pairs of nearest neighboring condensates in one-dimensional lattices. Eq.3 is equivalent to the bilinear-biquadratic spin chain model $\mathcal{H}/J = \cos \eta \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \sin \eta \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2$, if η satisfies $\tan \eta = (\alpha_1 - \frac{1}{3}\alpha_2 - \frac{2}{3}\alpha_0)/(\alpha_1 - \alpha_2)$ and the sign of $\sin \eta$ is chosen to be the same as that of $\alpha_1 - \frac{1}{3}\alpha_2 - \frac{2}{3}\alpha_0$.

The ground state of the bilinear-biquadratic Hamiltonian depends on η as suggested in [14]. The $\eta = 0$ point represents a usual $S = 1$ Heisenberg antiferromagnetic spin chain which was also studied in [15]. When η varies between $-3\pi/4$ and $-\pi/4$, one expects that the ground state of coupled condensates should be a dimerized valence-bond crystal, or DVBC.

As c_s defined after Eq.2 varies from 0 to $+\infty$, η varies from η_0 to $-\pi/2$; $\eta_0 = -\pi/2 - \arctan 1/2$. For spin-one bosons such as sodium atoms, c_s is much smaller than unity and our calculation shows that $\eta (\approx \eta_0)$ is precisely within the dimerized regime. This is further supported by a direct mapping between the problem of interacting spin-one bosons and a quantum dimer model (see below and Ref.16 for more discussions); it is also consistent with destructive interferences between Z_2 instantons in one-dimensional lattices for an odd number of atoms per site [16]. A straightforward calculation yields that the energy per site of a DVBC state is $\frac{E}{J} = -[\frac{5}{9}(\alpha_0 + \frac{\alpha_2}{2}) + \frac{\alpha_1}{6}]$, with $\alpha_{0,1,2}$ given in Eq.2.

In a dimerized configuration shown in Fig.1b), each two neighboring condensates are in a spin singlet state, or form a *valence bond*; this results in a valence bond crystal doubling the period of the underlying optical lattices. A DVBC state can be considered as a projected BCS pairing state of *pseudo-particles* introduced above. For one-dimensional lattices of $2M$ ($M \rightarrow +\infty$) sites with a periodic boundary condition, a DVBC state reads (up to a normalization factor)

$$|g\rangle = \mathcal{P}_{G.G} \mathcal{P}_{2M} \exp \left(\sum_{\alpha=0,1} g_\alpha \Psi^+(Q_0 = \alpha\pi) \right) |0\rangle \quad (4)$$

where $\Psi^+(Q_0) = \frac{1}{\sqrt{V_T}} \sum_Q \frac{h(Q)}{\sqrt{3}} [A_{Q,1}^+ A_{-Q+Q_0,-1}^+ + A_{-Q+Q_0,1}^+ A_{Q,-1}^+ - A_{Q,0}^+ A_{-Q+Q_0,0}^+]$. We have introduced

$A_{Q,m}^+$ as a bosonic creation operator of a spin-one *pseudo-particle* with a crystal momentum Q and $m = 0, \pm 1$; $h(Q) = \exp(iQ)$ and $Q \in [-\pi, \pi]$. $g_0 = 1, g_1 = \pm 1$ correspond to two-fold degenerate DVBC states [17]. $\mathcal{P}_{G.G.}$ is a generalized Gutzwiller projection to forbid a double or higher occupancy of *pseudo-particles* at each site and \mathcal{P}_{2M} is a projection into $2M$ -particle states. Eq.4 represents a projected superposition of singlet pairing states in $(Q, -Q)$ and $(Q, \pi - Q)$ channels. It appears to be plausible to observe interference between these two channels [18].

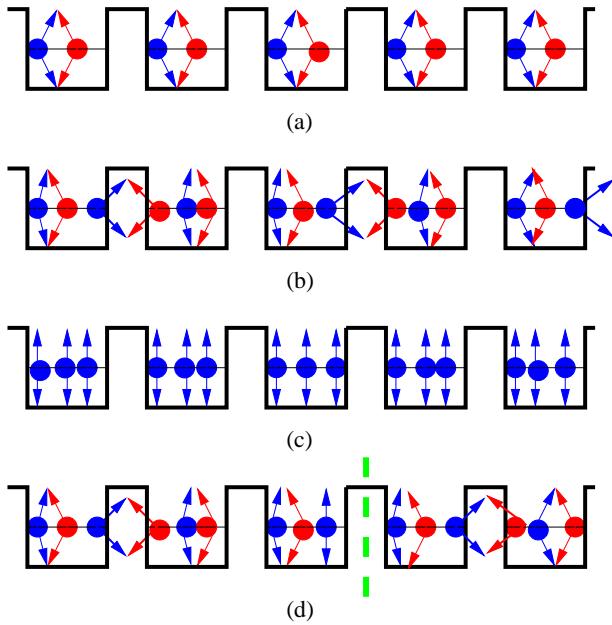


Fig.1 Schematic of microscopic wave functions for different one-dimensional Mott insulating states of spin-one atoms. a) A spin singlet Mott state for an even number of atoms per site; b) a DVBC Mott state for an odd number of atoms per site; as a reference, we also show in c) a nematic Mott insulating state which is stable only in high dimensional lattices [10]; d) a spin-one excitation (kink-like) in a DVBC state; the location of the kink is indicated by a green dashed line. In a), b), and d), each pair of blue and red dots represents a spin singlet state of two spin-one atoms. In c), d), a unpaired blue dot carrying an arrow pointing toward the direction of Ω represents an atom in a spin-one state specified by $\Omega = (\theta, \phi)$: $\frac{1}{\sqrt{2}} \sin \theta \exp(-i\phi)|1, 1\rangle - \frac{1}{\sqrt{2}} \sin \theta \exp(i\phi)|1, -1\rangle + \cos \theta|1, 0\rangle$; in c), localized atoms at each site "condense" in an identical spin-one state.

The DVBC state breaks the crystal translational symmetry and has a twofold degeneracy; one of the degenerate states is characterized by the following correlation functions ($i \neq j$)

$$\begin{aligned} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle &= -\frac{1}{4}(1 + (-1)^j)\delta_{j,i+1}, \\ \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle &= \frac{1}{16}(1 - (-1)^i)(1 - (-1)^j). \end{aligned} \quad (5)$$

Eq.5 indicates long-range order in valence bonds; the alternating feature between site $i = 2k + 1$ and $i = 2k$ in the correlation function reflects a two-fold degeneracy of DVBC states [19].

An $S = 1, S_z = m$ excitation can be created by the following product operator

$$C_{\gamma,m}^+ = \mathcal{P}_{G.G.} A_{\gamma,m}^+ \prod_{\xi \in \mathcal{C}_\gamma} [\Psi_\xi^+ + \Psi_\xi^-] \quad (6)$$

where $\Psi_\xi^+ = \frac{1}{\sqrt{3}}(A_{i,1}^+ A_{j,-1}^+ + A_{i,-1}^+ A_{j,1}^+ - A_{i,0}^+ A_{j,0}^+)$ is a creation operator of a valence bond at link ξ which connects two neighboring sites i and j ; $A_{\gamma,m}^+$ is the creation operator of a pseudo-particle or a collective state at site γ with spin $S = 1, S_z = m$. Finally, the product is carried over all links ξ along path \mathcal{C}_γ which starts at site γ and ends at the infinity; furthermore, \mathcal{C}_γ is chosen such that the first link along the path is occupied by a valence bond. Eq.6 also represents a spin-one domain wall soliton(of $S_z = 0, \pm 1$) located at site γ in the DVBC as shown in Fig.1d). Taking into account the hopping matrix of the domain wall $T_{ij} = -\frac{1}{3}\alpha_0[\delta_{i,j-2} + \delta_{i,j+2}]$ along one-dimensional lattices, we obtain the following band structure for spin-one excitations:

$$E(Q_x) = J\alpha_0\left(1 - \frac{2}{3} \cos 2Q_x\right) \quad (7)$$

with Q_x defined as a crystal momentum of the excitation, $-\pi/2 < Q_x < \pi/2$. These excitations are purely magnetic and involve no extra atoms, i.e. they are "neutral".

1D lattices with non-integer numbers of bosons per site When the number of bosons per site deviates from an integer, extra bosons can hop along one-dimensional lattices and form a superfluid state. The situation with $N_0 = 2k \pm \epsilon$, $\epsilon \ll 1$ is particularly simple. In this case, $2k$ spin-one bosons localized at each site are in a spin singlet state; extra bosons added to or removed from the system tend to condense in a state with zero crystal momentum. However, hyperfine spin dependent scatterings destroy spin long-range order of condensed spin-one bosons in one dimension as pointed out in [9,11]. The ground state therefore is spin disordered but phase coherent, similar to that in one-dimensional traps. Interactions between bosons furthermore lead to usual Bogoliubov quasi-particles with a sound-like spectrum as well as gapped spin-one spin-wave excitations.

To facilitate discussions on the case of $N_0 = 2k + 1 \pm \epsilon$, we introduce, besides spin-one "neutral" excitations, "charged" spinless domain-wall excitations. A "charged" excitation with a positive or negative charge (\pm) is defined by creation operator $B_{\gamma,\pm}^+$ and

$$C_{\gamma,m}^+ = \psi_{\gamma,-m} B_{\gamma,+}^+ = \psi_{\gamma,m}^+ B_{\gamma,-}^+ \quad (8)$$

where $\psi_{\gamma,m}^+(\psi_{\gamma,m})$ is a creation (annihilation) operator of a spin-one atom with $S_z = m$. Following Eqs.4,8, as it is added to one-dimensional DVBCs, a spin-one boson fractionalizes into a spin-zero domain wall (with an extra atom thus "charged") and a spin-one "neutral" domain wall because of a two-fold degeneracy at $N_0 = 2k + 1$. This is reminiscent of the physics in conducting polymers [20]. At $N_0 = 2k + 1 \pm \epsilon$, both types of domain walls are free quasi-particles and charged domain walls can condense at the bottom of a band similar to that in Eq.7, as a consequence of spin-"charge" separation in one-dimensional optical lattices. Spin-charge separation was previously pointed out for correlated electrons in antiferromagnets [21].

Disordered states in square lattices In the limit when $E_{c,s}$ are much larger than t , our analysis suggests that the constrained quantum rotor model (in Eq.1) generalized to square lattices should be equivalent to an Ising gauge theory in (2+1)D in a quantum spin-disordered limit (for detailed discussions on the mapping, see [16]). The effective Hamiltonian is (in an arbitrary unit) $\mathcal{H}_{p.c.} = -\Gamma \sum \sigma_x - \sum_{\square} \prod_{\square} \sigma_z$, where σ_x and σ_z are Pauli matrices defined at each link and \square stands for an elementary plaquette in square lattices in this case. The Hilbert space of $\mathcal{H}_{p.c.}$ is subject to a local constraint $\prod_{\square} \sigma_x = (-1)^{N_0}$ at each site, with the product carried over all links connected with that single site. In (2+1)D, this Ising gauge field model $\mathcal{H}_{p.c.}$ is dual to an Ising model (frustrated when N_0 is an odd integer) in a transverse field and also represents a parity conserved quantum dimer model [22–27]. The frustrated Ising gauge field theory has been employed to investigate electron bond ordering [24–28].

As t becomes much smaller than E_s , Γ approaches infinity. By examining the model straightforwardly, one finds that the ground state of $\mathcal{H}_{p.c.}$ for $N_0 = 2k$ is a non-degenerate spin singlet; this is consistent with previous discussions on Mott states for an even number of atoms. For $N_0 = 2k + 1$ and $\Gamma \gg 1$, the ground state breaks no continuous symmetries but does break the lattice translational symmetry. It has a four-fold degeneracy and supports no gapless modes. This result implies that in a square lattice in a quantum spin disordered limit, the ground state for an odd number of bosons per site should be a valence-bond crystal (columnar-type) state. Two dimensional valence-bond crystals have also been proposed in a few recent models on strongly-correlated electrons [25–27] and in earlier works [29,30,28,24,31].

The ground state $|g\rangle$ on a torus of $2M \times 2M$ sites should be topologically identical with one of the following configurations

$$\mathcal{P}_{G,G} \mathcal{P}_{4M^2} \exp \left(\sum_{\eta,\xi=0,1} g_{\eta\xi} \Psi^+(\mathbf{Q}_0 = (\eta\pi, \xi\pi)) \right) |0\rangle. \quad (9)$$

In Eq.9, $g_{11} = 0$, $g_{00} = \pm g_{10} = 1$, $g_{01} = 0$, $\Psi^+(\mathbf{Q}) = \exp(i\mathbf{Q} \cdot \mathbf{e}_x)$ and $g_{00} = \pm g_{01} = 1$, $g_{10} = 0$, $\Psi^+(\mathbf{Q}) = \exp(i\mathbf{Q} \cdot \mathbf{e}_y)$ correspond to four-fold degenerate DVBC states in square lattices ($\Psi^+(\mathbf{Q}_0)$ is defined after Eq.4).

An examination of Eq.9 indicates that both "charged" spinless solitons and spin-one "neutral" solitons similar to those introduced in one-dimensional lattices interact with each other via a linear confining potential in a two-dimensional DVBC. The ground state therefore supports excitations of $S = 2, 1$ bound states of soliton anti-soliton pairs unlike in one-dimensional DVBC states.

We should emphasize here the important differences between the physics of Mott insulating states of interacting spin-one bosons and of Heisenberg antiferromagnets (unfrustrated). First, for interacting spin-one bosons, the Hilbert space at each site involves different spin states ($S = 1, 3, 5, \dots$ for an odd N_0 much larger than unity) unlike in Heisenberg antiferromagnets; this leads to a unique Ising gauge symmetry in the problem of interacting spin-one bosons [9,11], nematic Mott states in high dimensional optical lattices [10] and dimerization in low dimensional Mott insulating states. Second, phase transitions between nematic and spin singlet Mott insulators for spin-one bosons can be conveniently investigated by changing exchange interactions between two sites or practically by tuning laser intensities in optical lattices. This opportunity appears to be absent in simple unfrustrated Heisenberg anti-ferromagnets.

Finally, we notice that two-fold degenerate states in one dimensional optical lattices could be qubits of a quantum computer. I would like to thank F. D.M Haldane for many stimulating discussions on the BLBQ model, E. Demler for an early collaboration on a related subject and the year 2001 workshop on "beyond BEC" at Harvard-MIT center for ultracold atoms for its hospitality. I am also grateful to Bianca Y. L. Luo for encouragement and support. This work is supported by the foundation FOM, in the Netherlands under contract 00CCSPP10, 02SIC25 and by NWO Projectruimte 00PR1929.

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